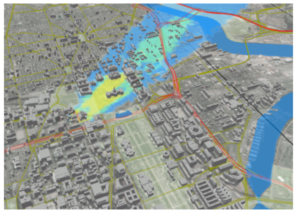
Los Alamos NATIONAL LABORATORY EST. 1943

Chemical Dense Gas Modeling Around Buildings Using the QUIC Model

Fall AGU Meeting 2007
LA-UR-07-3182

What is QUIC?

The Quick Urban & Industrial Complex (QUIC) dispersion modeling system

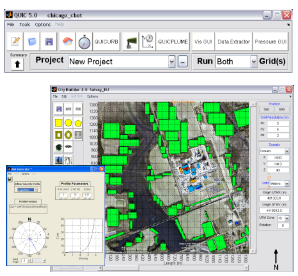


DC Mall tracer dispersion simulation

QUIC is comprised of:

* QUIC-URB
  produces 3D wind field around buildings using an empirical/diagnostic model
* QUIC-PLUME
  accounts for building-induced turbulence through a Lagrangian random-walk dispersion model
* QUIC-GUI
  graphical user interface for set-up, running, and visualization (QUIC-GUI)

The QUIC Graphical User Interface



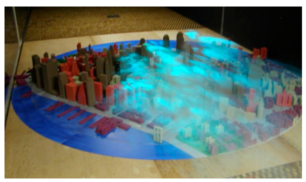
The QUIC-GUI allows for the user to easily set-up building layouts, specify the winds, choose a CBR agent type, and pick a release location.

2D and 3D visualization tools allow the user to rapidly display wind flow and plume dispersion patterns.

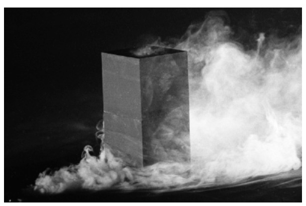
What is the Threat?

Large quantities of toxic chemicals are stored at numerous industrial sites around the country and shipped in large volumes via rail and roadways. Accidental releases are relatively common and there is also concern that terrorists could sabotage storage containers. Chemical releases are often heavier than air and stay close to the ground at high concentration.

Why Buildings?



Buildings can enhance lateral spread. The smoke released from a small surface-level source rapidly broadens down side streets. USEPA wind tunnel experiment from Heist et al. (2004).



Buildings enhance vertical spread. This image shows smoke being lofted high into the air by a tall building. BRE experiments from David Hall.

The consequences from a dense chemical gas in a city could be catastrophic. But no one is really sure how the dense gas will disperse. Will mixing be enhanced by buildings or will the toxic cloud become trapped between the buildings?

Dense Gas Scheme

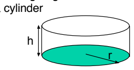
Instantaneous Source Representation

$$Volume_{dg} = \frac{Q}{\rho_{dg}}$$

$$Volume_{cylinder} = \pi \cdot r^2 \cdot h$$

$$r = \sqrt{\frac{Q}{\rho_{dg} \pi h}}$$

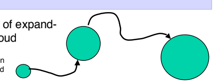
User specifies: h, Q, & ρ_{dg}
QUIC calculates r and uniformly distributes Lagrangian markers within a cylinder



Cloud Movement

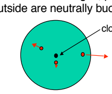
Track movement of expanding dense gas cloud

Cloud velocity based on volume average of wind field inside cloud



Dense Gas Outflow Velocities

Any particles inside the cloud behave as dense gas, particles outside are neutrally buoyant

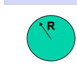


Outward buoyancy-driven velocity

$$\vec{V}_{dg} = \frac{dR}{dt}\frac{r_p}{R}$$

R = radius of cloud
r_p = distance from center of cloud

Cloud Growth Rate



$$\frac{dR}{dt} = \frac{1}{R}\sqrt{g\frac{\rho_{dg0} - \rho_a}{\rho_a} Vol_0},$$

$$\Delta Vol = (\pi R^2)(0.65 u_{*dg})\Delta t + (2\pi R h)(0.7\frac{dR}{dt})\Delta t$$

entrainment thru top
entrainment thru sides

$$h = \frac{Vol}{\pi R^2}$$

From Hanna and Drivas (1987)

Turbulence Damping

$$u_{*dg} = \frac{u_*}{(1 + 0.2 \cdot Ri_\#)}$$

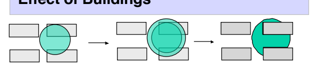
where $Ri_\# = gh\frac{\rho_{dg} - \rho_a}{\rho_a u_*^2}$

$$\sigma_{u_i dg} = \sigma_{u_i}\frac{u_{*dg}}{u_*}$$

Small random vertical perturbations added to keep particles well-mixed within dense cloud

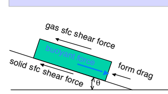
From Briggs, Britter, Hanna, Havens, Robins, and Snyder (2001)

Effect of Buildings



Compute an "effective" radius based on volume occupied by buildings

Effect of Topography



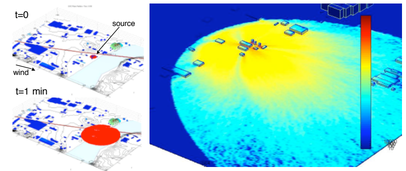
Based on force balance

Slug Velocity

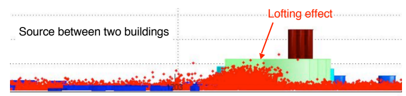
$$V = \left[\frac{\left(g\frac{\rho_{dg} - \rho_a}{\rho_a}H\right)\sin\theta}{2\frac{\rho_{dg}}{\rho_a}\left(\frac{u_*}{U}\right)^2 + \frac{H}{\pi R}C_D}\right]^{1/2}$$

From DeNevers (1984)

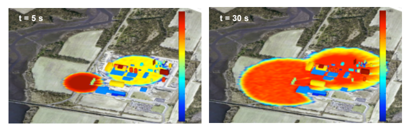
Dense Gas Simulations



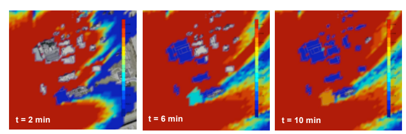
QUIC simulation of a dense gas chlorine release at an industrial facility. Left: particles at initial time and one minute later illustrating the dense gas slumping effect. Right: the deposition field shows that heavier-than-air releases can have significant crosswind and upwind transport.



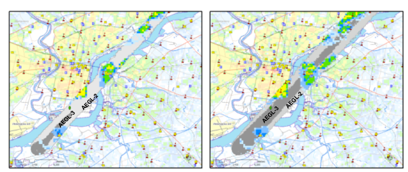
A side-view showing that the dense gas cloud generally remains low to the ground. However, near buildings, the dense gas is lofted higher into the air, resulting in lower surface concentrations.



Left: a near-instantaneous gaseous release and a liquid pool evaporating source. Right: the clouds merge after a short time.



Infiltration calculations of outdoor vs. indoor toxicity levels, helpful for estimating the time onsite personnel would have to respond.



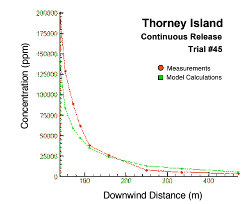
Simulations are used to estimate potential impacts to the populace. Location of indoor (left) and outdoor (right) population that may need medical care (i.e., impacted at AEGL-2 and 3 dosage levels).

How accurate is QUIC?

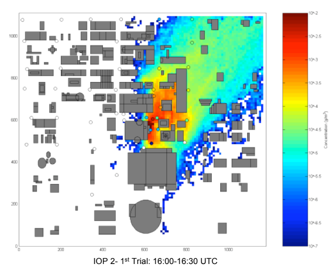
QUIC has been tested against both field and lab tracer data, as well as buoyant rise experiments. QUIC will never give perfect answers, but it will account for the effects of buildings in an approximate way and provide more realism than non-building-aware dispersion models.

6 Different Codes - Output Range:			
Concentration [ppm]:	2000	400	20
Max. Distance [km]:	0.66-1.8	1.8-4	10-20
QUIC [km]	0.76	1.8+	15.2

Comparison of QUIC to six other dense gas dispersion models for a chlorine release over flat terrain.



Validation of the QUIC dense gas module using Thorney Island field data.



Plume dispersion comparisons with Oklahoma City Joint Urban field data (filled circles).

QUIC is a fast response urban dispersion model that runs on a laptop. Versions are available for Windows, Mac, and Linux OS's. CBR agent dispersion can be computed on building to neighborhood scales in tens of seconds to minutes.

The code is being used to assess the consequences of dense gas releases. It is being used to scope the magnitude of health impacts, to develop rules-of-thumb for emergency responders, and to create mitigation strategies for industrial facilities.

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